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THE PESTICIDE ROOT ZONE MODEL (PRZM): A PROCEDURE FOR EVALUATING PESTICIDE LEACHING THREATS TO GROUNDWATER

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ABSTRACT

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INTRODUCTION

Pesticide leaching from agricultural fields has lead to groundwater contamination (Peoples et al., 1980; Rothenschild et al., 1982; Zaki et al., 1982;

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Wehtje et al., 1983. The potentially widespread nature of resulting contamination makes remedial actions difficult because there is no single plume eminating from a 'point source' (the more common groundwater problem) that can be isolated and controlled. In any case, a more prudent approach to prevention or reduction of groundwater contamination by pesticides must be based on understanding the relationships among chemical properties, soil system properties, and the climatic and agronomic variables that combine to induce leaching. Knowledge of these relationships can allow a priori investigation of conditions that lead to problems and appropriate actions can be taken to prevent widespread contamination. This paper describes the Pesticide Root Zone Model (PRZM), a mathematical simulation technique that has been developed (and partially tested) to evaluate pesticide leaching potential under field crop conditions.

Many investigators have studied the factors contributing to pesticide leaching (Davidson et al., 1975; Wood and Davidson, 1975; Stewart et al., 1976; Selim et al., 1977; Enfield et al., 1983). Their investigations have shown that chemical solubility in water, sorptive properties, pesticide formulation, and soil persistence determine pesticide leaching. Similarly, the important environmental and agronomic factors include soil properties, climatic conditions, crop type, water management methods, and cropping practices. Many of the environmental factors are highly time-variable and soil properties are spatially variable. In short, the hydrologic cycle interacts with the chemical properties and characteristics to transform and transport pesticides within and out of the soil profile. Vertical movement out of and below the root zone can result in ground water contamination.

The need for accelerated development of models to evaluate leaching is supported by prevailing production trends in the pesticide manufacturing industry. Table 1 illustrates a growing movement toward production of more soluble (and hence more leachable) compounds for use as insecticides.

Modeling solute transport in soil systems and other porous media is not new. Numerical models for the movement of solutes in soil columns for steady-state, transient, homogeneous, and multi-layered conditions have been developed (Davidson et al., 1975; Wood and Davidson, 1975; Selim et al., 1977; Gureghian et al., 1979). Included in such studies have been linear and nonlinear sorption, ion exchange, and other chemical-specific reactions. These investigations have proven valuable in interpreting laboratory data, investigating basic transport processes, and identifying controlling factors in transport and transformation. As noted in a recent review of models for simulating the movement of contaminants through ground water (Anderson, 1979), however, the successful use of such models will require a great number and variety of detailed field data. This unfortunate conclusion arises from the scaling problems associated with laboratory experiments and the tradi-

TABLE 1

Water solubilities of representative insecticides by class *

Class	Major period of development	Common name (U.S.A.)	Water (20–25°C) solubility (mg/l)
Organochlorine	1940–1960	Aldrin	0.025
		Alpha-endosulfan	0.530
		Chlordane	0.0090
		DDT	0.0012
		Dieldrin	0.25
		Endrin	0.23
		Heptachlor	0.056
		Lindane	10.0
		Methoxychlor	0.1
		Toxaphene	3.0
Organophosphate	1960–1970	Azinphos-methyl	29.0
		Diazinon	40.0
		Disulfoton	2.5
		Ethoprop	750.0
		Fenitrothion	20.0
		Malathion	150.0
		Methyl parathion	55.0
		Parathion	24.0
		Phorate	50.0
Carbamate	1970–present	Aldicarb	6000
		Aldicarb sulfoxide	28000
		Aldoxycarb	7800
		Carbofuran	700
		Fenamiphos	400
		Fosthietan	5000
		Methomyl	58000
		Oxamyl	280000

* Gunther et al. (1968), Union Carbide Corporation (1975), Roberts et al. (1977) and Calahan et al. (1979).

tional solution of the appropriate partial differential equations at points or nodes in a finite-difference or finite-element grid network. Each spatial segment modeled must be properly characterized. The inherent spatial variability of most field soils renders this characterization a difficult and expensive, if not impractical, task.

Such real problems in modeling pesticide leaching with existing procedures are discouraging when one considers the need to evaluate future problems arising from pesticides not yet widely distributed or used. Indeed, some investigators have proposed stochastic modeling approaches to accom-

modate the spatial variability (Peck et al., 1977; Dagan and Bresler, 1979; Warrick and Amoozegar-Fard, 1979). Models designed to evaluate or screen potential problems should conform to the maximum possible extent to known theory but must be structured to enable efficient analysis of field situations with minimal requirements for specialized field data. In short, the goal is to integrate the essential chemical-specific processes for leaching with reasonable estimates of water movement through soil systems. Data input requirements are to be reasonable in scope and generally available from existing data bases.

A MATHEMATICAL STATEMENT OF THE PROBLEM

The interactions of pesticides and soil–water–plant systems include surface runoff (in water and on eroded sediment), advection in percolating water, molecular diffusion, dispersion, uptake by plants, sorption to soil particles, volatilization, biological degradation, and chemical degradation. If a surface zone characterized by erosion and runoff losses is distinguished from subsurface zones where only vertical movement is allowed mass balance equations of one dimension can be derived for both solution and sorbed phases of a pesticide. The further assumption of linear, reversible, and instantaneous equilibrium sorption yields, for the surface zone:

$$\frac{\partial(C_w\theta)}{\partial t} = \frac{\partial D}{\partial x}\frac{\partial(C_w\theta)}{\partial x} - \frac{\partial(vC_w\theta)}{\partial x} - k_u T C_w - \mathrm{RO}\, C_w - \sum k_w C_w\theta + F_d J_{ap}; \quad 0 \leqslant x \leqslant X \tag{1}$$

$$\frac{\partial(C_s\rho)}{\partial t} = -\mathrm{ERO}\, C_s - \sum k_s C_s\rho + (1 - F_d) J_{ap} \tag{2}$$

where C_w = dissolved pesticide concentration in soil water (ML^{-3}); C_s = sorbed pesticide concentration (MM^{-1}); θ = soil volumetric water content (L^3L^{-3}); ρ = soil bulk density (ML^{-3}); D = coefficient of dispersion and diffusion (L^2T^{-1}; v = water pore velocity (LT^{-1}); k_u = pesticide plant uptake efficiency, $0 \leqslant k_u \leqslant 1.0$; T = plant transpiration rate (LT^{-1}); RO = volumetric rate of surface water runoff (L^3T^{-1}); k_w = summation of all first-order rate constants for transformation of dissolved pesticides (T^{-1}); F_d = fraction of applied pesticide in dissolved form; J_{ap} = pesticide application rate (MT^{-1}); t = time (T); x = vertical distance (L); X = depth of surface runoff zone (L); ERO = surface soil erosion rate (MT^{-1}); and k_s = summation of all first-order rate constants for transformation of sorbed pesticides (T^{-1}). For the lower subsurface zones:

$$\frac{\partial(C_w\theta)}{\partial t} = \frac{\partial D}{\partial x}\frac{\partial(C_w\theta)}{\partial x} - \frac{\partial(vC_w\theta)}{\partial x} - k_u T C_w - \sum k_w C_w\theta \tag{3}$$

$$\frac{\partial(C_s\rho)}{\partial t} = -\sum k_s C_s \rho; \quad X \leqslant x \leqslant \infty \tag{4}$$

For both cases the linear interaction term for sorbed and dissolved phases is:

$$C_s = K_p C_w \tag{5}$$

where K_p = partition coefficient (L^3M^{-1}).

It also is convenient, if not required by the experimental methods most often used to estimate transformation rate constants, to use the equality $\Sigma k_w = \Sigma k_s = \Sigma k$.

Equations (1–5) can be combined to yield basic equations for each zone written in terms of the dissolved pesticide concentration, C_w.

$$\frac{\partial(C_w(\theta + K_D\rho))}{\partial t} = \frac{\partial D}{\partial x}\frac{\partial(C_w\theta)}{\partial x} - \frac{\partial(vC_w\theta)}{\partial x} - C_w(k_u T + K(\theta + K_D\rho) + \mathrm{RO} + \mathrm{ERO}\, K_D\rho) + J_{ap} \tag{6}$$

where

$\mathrm{RO} = \mathrm{RO}$ for $0 \leqslant x \leqslant X$

$\mathrm{ERO} = \mathrm{ERO}$

and

$\mathrm{RO} = 0$ for $X \leqslant x \leqslant \infty$

$\mathrm{ERO} = 0$

Equation (6) is a variation on the advection–dispersion model most often derived as the basis for ground water quality models. The plant uptake term, represented here as a simple linear function of plant transpiration, is not included in most representations and the runoff and erosion terms are rarely included. Equation (6) could be modified further to include the influence of a vapor phase pesticide component following the approach of Jury et al. (1980). For many very soluble pesticides, however, voltalization from within the soil profile is not a major mode of less (Burkhard and Guth, 1981).

Most solutions to eq. (6) (without runoff, erosion, and uptake included) have been numerical because the velocity, v, and soil moisture content, θ, are both functions of time, t, and distance, x. Assumptions of constant velocity and moisture content have been made by some investigators to enable development of analytical solutions. Specifically, for pesticides Enfield and Carsel (1980) have obtained such a solution when v is both constant and known. For other situations, analytical solutions remain untractable and in any case v and θ must be known or modeled.

Because v and θ are not generally known and not generally measured as part of routine monitoring programs, it is necessary to develop additional equations for these variables. In general case Darcy's law can be combined

with the continuity equation to yield:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{(\partial \phi)}{\partial x} \right) \tag{7}$$

where k = hydraulic conductivity; ϕ = hydraulic potential; and:

$$v = -k\ \partial \phi / \partial x \tag{8}$$

For the general case, eqs. (6–8) must be solved as coupled equations. However, when the solute concentrations are quite low and do not influence flow, then the solute transport and flow equations can be decoupled.

Equations (6–8) can be solved numerically. Gureghian et al. (1979) obtained such a solution and performed sensitivity analyses that can give valuable insight into the leaching process. In their study, the movement of nitrogen in soil columns was investigated under transient, steady-state, and multi-layered soil conditions. Earlier Davidson et al. (1975) developed numerical models for simultaneous water and solute movement in soil profiles. Pesticides were used as solutes in the study and different sorption models were investigated for their utility in explaining the observed concentration profiles. More recently Enfield et al. (1983) obtained steady-state solutions for eq. (6) for specified values of flow velocities and flow volumes (recharge). Lacking in all these approaches is accommodation of the infiltration processes at the soil surface, removal of soil moisture by evapotransposition, plant uptake, variable chemical application times and amounts, and mass balance accounting for runoff losses. Inclusion of all the above processes in the simultaneous solution of eqs. (6–8) is difficult for several reasons. First, the equations are written for vertical movement at a point, but field soils are quite variable and conditions at one point may not be representative of other points. This spatial variation is mathematically treated by solving the equations in two or three dimensions but the problem remains to characterize the physical system being modeled. Second, the vertical characteristics of field soils are also highly variable and inputs required for eq. (7) may not be within economical reach. In addition, the hydraulic conductivity and pressure head versus moisture content relationships of some soils may not be single-valued functions. Indeed, in a review of ground water modeling, Anderson (1979) noted that the scarcity of field data and the lack of appropriate measurement techniques remain as obstacles to routine application of models (advection–dispersion–Darcian) to solve contaminant transport problems. Thus, mathematical solution of eqs. (6–8) by numerical methods does not necessarily lead to an effective tool for evaluating pesticide leaching risks to ground water. Such solutions are valuable in developing fundamental insights into the governing processes to be sure, but the goal remains to develop an operational procedure for leaching assessment.

Before proceeding in developing a solution, it is useful to reconsider the pesticide leaching problem. Pesticide leaching from field-sized areas is the major concern. Because most pesticides are applied on, just beneath, or near the soil surface, the rainfall–infiltration–runoff process must be described. Movement within and below the root zone is influenced by soil moisture, which requires continuous soil moisture accounting in the model. Various field crops are of interest each having different growth patterns, rooting depths, and transpiration requirements. Pesticide transformation process parameters (e.g., kinetic rate constants) may vary with soil depth as well as moisture and other variables so that dispersion and advection have important interactions with transformation processes. Superimposed on these factors is the objective to develop efficient, reasonably accurate solutions obtained from data generally available from national data bases, maps, and field handbooks.

Equation (6) can be solved numerically if for each time step the moisture content, θ, and pore velocity, v, are also known. Furthermore, if 'field-averaged' values for θ and v are estimated, then the solution is no longer restricted to only a point value. In this manner a pseudo-three dimensional solution is obtained with spatial averages for two dimensions. The accuracy of this approach is quite sensitive to the distribution function that describes the field spatial variability. Existence of skewed, non-normal distributions will influence the expected value for leaching and must be acknowledged and accommodated where possible.

Mass balance equations for water in each of three kinds of soil layers can be written as follows:

— surface layer:

$$\mathrm{SW}_{1,t+1} = \mathrm{SW}_{1,t} + P_t + \mathrm{SM}_t - \mathrm{INT}_t - R_t - E_{1,t} - \mathrm{PER}_{1,t} \tag{9}$$

— root zone layers:

$$\mathrm{SW}_{i,t+1} = \mathrm{SW}_{i,t} + \mathrm{PER}_{1,t} - E_{i,t} - T_i - \mathrm{PER}_{i-t} \tag{10}$$

$2 \leqslant i \leqslant \sup(i)$ for the root zone layer

— below root zone layers:

$$\mathrm{SW}_{i,t+1} = \mathrm{SW}_{i,t} + \mathrm{PER}_{i-t} - \mathrm{PER}_{i,t} \tag{11}$$

$\sup(i) < i \leqslant$ total number of soil layers for the root zone layer

where $\mathrm{SW}_{i,t}$ = soil water in layer i for day t (cm); INT_t = interception of precipitation by plants for day t (cm); INFIL = infiltration for day t (cm); E = evaporation for day t (cm); T = transpiration for day t (cm); PER_t = percolation of soil water from zone i for day t (cm).

The 'field-averaged' results arise from the way each of the above terms are estimated. Infiltration is the key variable and is determined as:

$\text{INFIL} = P - R$ for rainfall

or

$\text{INFIL} = \text{SM} - R$ for snowmelt conditions

where P = precipitation as rainfall (cm); R = surface runoff (cm); SM = snowmelt. The runoff term, R, is estimated from the well-known USDA Soil Conservation Service (SCS) curve number method and is implemented in PRZM in a manner similar to the approach taken in current pesticide runoff models. Snowmelt is estimated by the degree-day approach also included in many runoff models. Details are provided in Knisel (1980), Mockus (1972), Haith and Loehr (1979) and Stewart et al. (1976). The total runoff calculation estimated using this approach will produce, in turn, an estimate of the total infiltration for the field. Thus, a 'lumped average' representation of the field's infiltration is used as the input to solution of eq. (6). The spatial distribution of this infiltration is not known, however, and thus PRZM is not expected to exactly reproduce conditions (e.g., pesticide concentration profiles) at any single point.

Total evapotranspirative demand is estimated as:

$$E_i + T_i = \text{SMFAC}_i * \text{PET}_i \tag{12}$$

where SMFAC_i = soil moisture factor; and PET_i = maximum potential evapotranspiration (cm). This total demand is divided into soil evaporation and plant transpiration. The demand is substracted sequentially from each layer until a minimum moisture level is reached (designated as the wilting point) for each layer. Evaporation is assumed only to occur in the top 10 cm of the soil profile with the remaining demand, crop transpiration, occuring from below the 10-cm zone to the maximum depth of rooting. These assumptions, although admittedly somewhat arbitrary, allow simulation of reduced levels of evapotranspiration during the fallow, dormant periods and increased levels during active plant growth. The depth of the root zone varies during the year beginning at crop emergence and increasing in a step-wise manner until the maximum rooting depth is achieved at crop maturity. Values for SMFAC and PET are reasonably well-known and can be determined readily from climatic data. Details are available in Haith and Loehr (1979).

The remaining term in eqs. (9–11) is the volume of percolating water, PER_i. In many ways this is the most troublesome variable to predict and unfortunately is the major determinant of leaching. In short, the volume of water percolating below the root zone is the upper limit of ground water recharge (it can be intercepted by impermeable layers or artifical drains) and

must transport the pesticide to the saturated, ground water zones. PER in this model is defined rather simply in the context of two bulk soil moisture holding characteristics commonly reported for agricultural soils: field capacity and wilting point. Field capacity is somewhat imprecise measure of soil water holding properties and is usually reported as the moisture contant that field soils attain after all excess water is drained from the system under influence of gravity. The difficulty with this concept is the fact that some soils will continue to drain for long periods of time and thus field capacity is not a constant. Given the lack of theoretical and physical riger, the concept remains as a useful measure of soil moisture capacity and has been success-

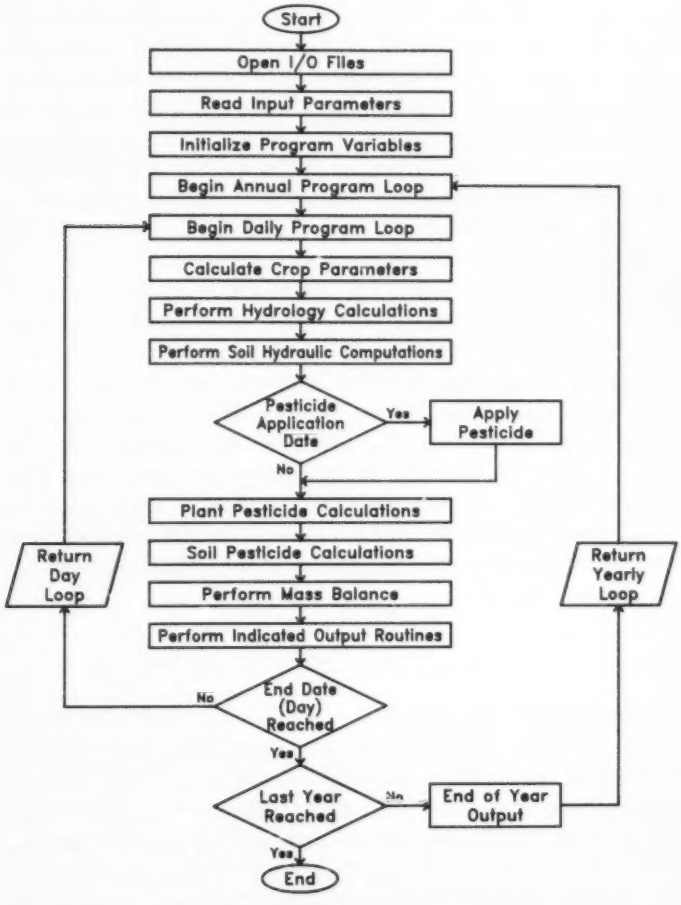

Fig. 1. Flow chart for PRZM model.

fully used in a number of water balance models (Stewart et al., 1976; Haith and Loehr, 1979). Wilting point of soils is a function of both soils and plants. It is defined as the soil moisture content below which plants are unable to extract water.

Field capacity and wilting point are used operationally to define two reference states in each soil layer for predicting percolation. If the soil water, SW, is calculated to be in excess of field capcity, then percolation, PER, is allowed to remove the excess water to a lower zone. The entire soil profile excess is assumed to drain within 1 day. The lower limit of soil water permitted is the wilting point. The difference between field capacity and wilting point is available to account for removal by evapotranspiration. One outcome of these assumed 'drainage rules' is that the soil layers below the root zone quickly reach field capacity and remain at that value. When this condition is reached, all water percolated below the root zone will displace the water within the lower soil layer simulated and so on. Such conditions may not occur in some soils and hence the emphasis on movement below the plant root zone is perhaps the most meaningful model output. Water balance accounting in this manner should be most accurate for sandy soils and is least accurate for tight, clay soils (Stewart et al., 1976). Fortunately, the greatest concern for leaching arises for sandy, loose soils.

Chemicals that leach to ground water are not likely to erode as sorbed pollutants to any large degree but an erosion term was included for completeness. A modification to the Universal Soil Loss Equation (USLE) was adopted for the purpose. Details are given by Williams and Berndt (1977).

Equation (6) was solved numerically by a backwards-difference, implicit scheme. Values for moisture content and velocity are provided by the decoupled solution of eqs. (9–12). The spatial dimension and time step chosen are functions of the accuracy desired. Sensitivity analyses were performed to evaluate these parameters and values of 5 cm and one day were selected as optimum for the purposes of the model. A flow chart showing the model structure is shown in Fig. 1.

MODEL TESTING

The operational use of screening models for evaluating pesticide threats to ground water should be built on a carefully designed and comprehensive model testing effort. Testing model concepts and comparing model simulations with laboratory or soil column data are useful excercises but clearly are not sufficient if field scale predictions are desired. In short, model performance testing using field data is essential. Toward that end, the U.S. Environmental Protection Agency's Environmental Research Laboratory, Athens, GA, has initiated a cooperative research project with the Georgia

District Office of the U.S. Geological Survey to develop field data for testing PRZM and for investigating spatial variability of pesticide leaching in field soils. Successful completion of this field project should provide a comprehensive data set for model testing. In the interim, however, data collected as part of a study of aldicarb in New York (INTERA, 1980) were used in evaluating the performance of PRZM.

Two kinds of performance testing are of interest: (1) tests using laboratory-derived chemical data and generally available environmental data for the site, and (2) tests using site-specific data for model calibration. Results from the first test are indicative of the accuracy expected when operating PRZM in a screening mode for assessment of pesticides not yet released into the environment. The second test results more clearly demonstrate the predictive capability of the model when local or site-specific variations (e.g., dispersion, soil properties) are accounted for.

The extent to which either kind of test can be performed is limited by the available data and the experimental design controlling field experiments. The spatial variability phenomenon presents a special problem in model testing that unfortunately can not be fully addressed in the testing reported here.

Summaries of the available chemical-specific data for aldicarb have been reported (Bromilow, 1975; Hough et al., 1975; Smelt et al., 1978a, b, c; INTERA Environmental Consultants, 1980; Pacenka and Porter, 1980). The range of values reported for both its sorptive and persistence characteristics is quite large: first-order rate constants varied from 0.0 to 0.1 day^{-1} and distribution coefficients from 0.073 to 0.34 l/mg. In general, a picture of a potentially long-lived, highly soluble compound emerges. The apparent first order rate constants are especially noteworthy. Aldicarb readily oxidizes to a sufoxide and sulfone (Smelt et al., 1978a, b, c; Union Carbide Corporation, 1983). Transformation to the oxidized form is quite rapid but further transformations are much slower. The aldicarb–sulfoxide–sulfone forms are all acetylcholinesterase inhibitors (Union Carbide Corporation, 1983). Thus the environmental problem is the combined, total concentration of the three species.

TABLE 2

Hydrologic summary for New York simulation

Year	Predicted			
	Rainfall (cm)	Runoff (cm)	Evapotranspiration (cm)	Recharge (cm)
1977	129	11	37	81
1978	128	12	36	80
1979	131	9	38	84

Modeling the combined concentrations as a single specie obeying a simple first-order rate equation requires further elaboration. In a general, rigorous sense such an approximation is incorrect; however, it is readily shown that if the partition coefficients are very small and if intermediate rate constants are quite large then the general solution reduces to a simple first order expression. Apparently this is precisely the case with aldicarb.

The hydrologic summary for the New York simulation is given in Table 2. There are no hydrologic data from the field site to verify the water balance components of PRZM. Certain observations can be made, however. The runoff total is small, only 8% of rainfall, and this is consistent with observations for the sandy soils of Long Island (Hoffman and Lubke, 1961). More importantly, the recharge water comprises a large fraction of rainfall, 63%. Hoffman and Lubke (1961) state that ground water recharge is approximately 50% of rainfall. The model may be overestimating recharge, and this could be due to an underestimation of evaporation (ET) demand. For the New York simulations, an empirical formula based on daily average temperature may have underestimated ET. ET is estimated more nearly correct when based on pan evaporation, because pan evaporation totals are a function of humidity, windspeed, temperature, and solar radiation.

The observed data for the New York study (INTERA, 1980) are presented as soil concentration profiles of total toxic residue (aldicarb + sulfoxide +

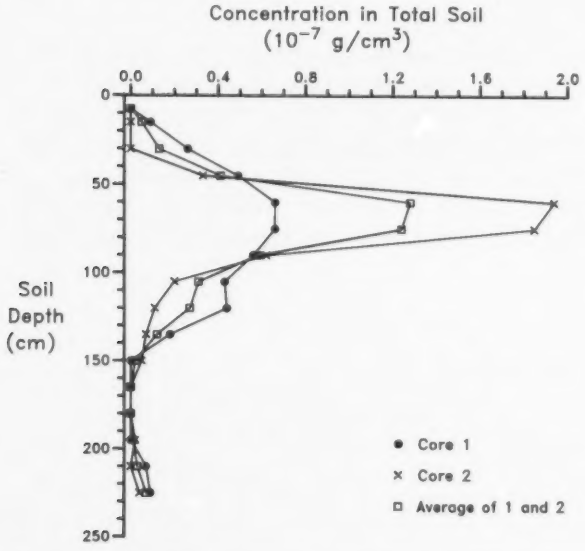

Fig. 2. Observed aldicarb (reported as sulfone) at New York site.

TABLE 3

Summary of site conditions and pesticide use for New York *

Model parameters				
Hydrology		Pesticide application		
		Year	Date	Rate (kg/ha)
Root zone depth (cm)	30.0	1977	4/15	2.24
Unsaturated zone depth (cm)	225.0	1977	6/10	1.35
Hydrologic classification	B	1978	4/14	2.52
Textural classification	Sandy loam	1978	6/10	2.02
Soil series designation	Haven	1979	4/15	3.19
Average field capacity (cm/cm)	0.24	1979	6/10	2.52
Average wilting point (cm/cm)	0.10			
Bulk density (g/cm^3)	1.50			
Meterologic station	Riverhead			
Average date of potato emergence	10 May			
Average date of potato maturity	10 August			
Average date of potato harvest	10 September			

* INTERA (1980) and Pacenka and Porter (1980).

sulfone) in Fig. 2. The spatial variability is obvious although insufficient data exist to characterize the nature of the variation. The peaks are located at approximately the same depth suggesting most of the variation is in the degradation rather than the transport. This seems quite reasonable given the uniformity of the deep sands found in the site (Pacenka and Porter, 1980). Note also the slight increase in the concentrations below 200 cm. This increase is thought to be the previous year's application of aldicarb (INTERA, 1980).

A comparison of the environmental conditions summarized in Table 3 and the experimental conditions for the experiments reported in the literature led to a choice of 'best' model parameters for the individual simulations. Two sets of degradation rate constants and partition coefficients are of interest — one set for the root zone (top 30 cm) and the second for a depth below the root zone but above the water table (30–225 cm). Model parameters for these conditions were $k = 0.014$ day^{-1}, $k_p = 0.146$ l/mg and $k = 0.0009$ day^{-1}, $k_p = 0.073$ l/mg, respectively.

A comparison of the observed and simulated concentration profiles using the literature-based model parameters is given in Fig. 3. This test result could be described as the 'calibration-free' performance of the model because local, site-specific measurements were not used in the model and sensitivity analyses were not performed to fine tune the modeling results.

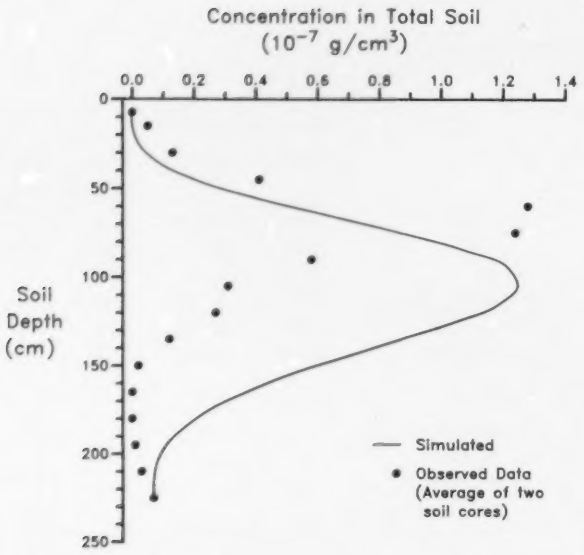

Fig. 3. Comparison between computed and observed aldicarb for the average of two soil cores at the New York site.

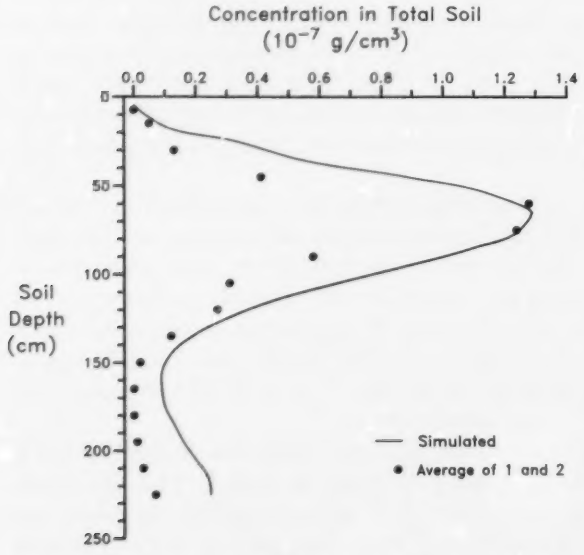

Fig. 4. Calibration results for the average of the two aldicarb cores at the New York site.

TABLE 4

Model parameters for pre-calibration and post-calibration results

	First-order rate	Lumped decay constant (day^{-1})	Partition coefficient (l/mg)	
	root zone	lower zone	root zone	lower zone
Selected literature-reported lab studies	0.014	0.0009	0.15	0.07
Calibrated values				
First core	0.016	0.002	0.30	0.15
Second core	0.008	0.002	0.30	0.15
Mean	0.012	0.002	0.30	0.15

The degradation rate constants appear to be most nearly correct but the simulated peak is deeper than the observed. The peak depth is determined from the volume of net water recharge and the retarded velocity of the solute resulting from sorption. The distribution of this error between the two processes in the simulated values is unknown.

Performance of hydrologically based pesticide fate and transport models can be dramatically improved by the calibration process (Lorber and Mulkey,

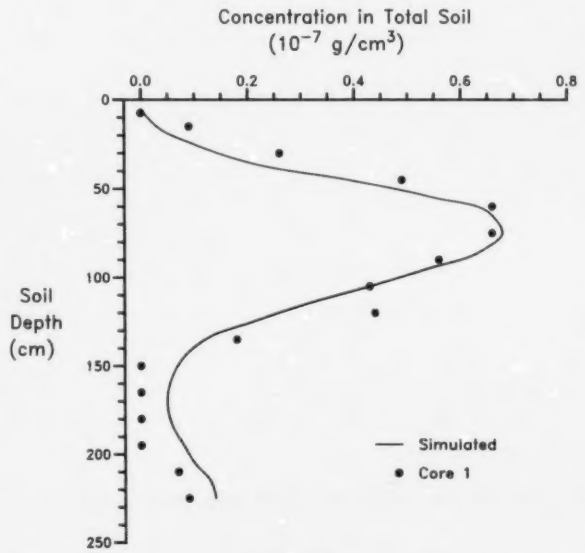

Fig. 5. Calibration results for aldicarb from core 1 at the New York site.

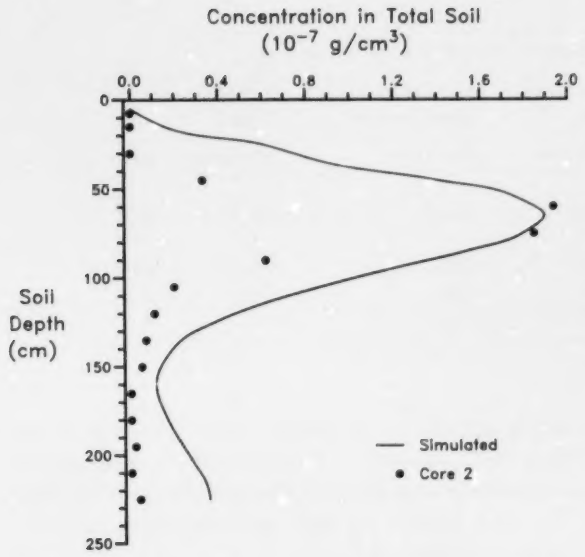

Fig. 6. Calibration results for aldicarb from core 2 at the New York site.

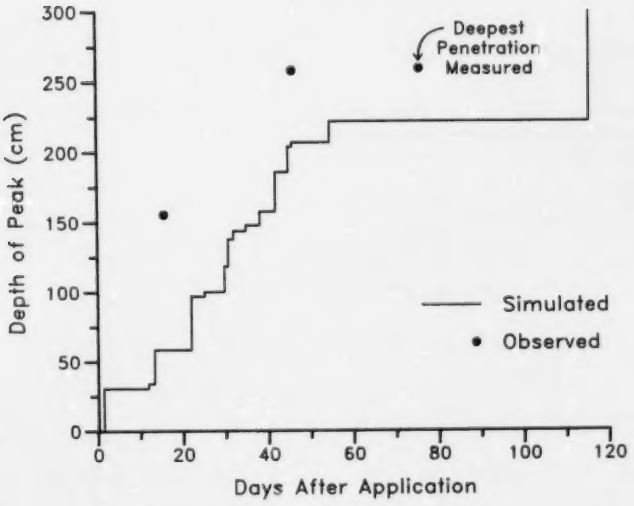

Fig. 7. PRZM test results for aldicarb use in citrus production (after Jones et al., 1983).

1982). Calibration simply adjusts the model parameters to more nearly approximate the prevailing site conditions. Caution must be exercised, however, to avoid calibrated parameter values that fall outside the measured range of such values. Calibration of PRZM at the New York site was completed for each soil core and for mean values. The resulting calibrated model parameters and the literature-lab values used previously to produce the 'calibration-free' results of Fig. 3 are given for comparison in Table 4. The observed and simulated concentration profiles are shown in Figs. 3–6. The calibrated model parameters are all within the reported range of measured values suggesting the PRZM is effectively modeling the relevant processes operating on the pesticide.

The results summarized in Figs. 3–6 are encouraging but do not constitute a rigorous performance test of the model. For example, the calibration enabled a better match of the peak location by varying the partition coefficient and hence the vertical velocity of the pesticide. Because only limited data on the hdrology of the area were available, no adjustments were made that would change the recharge estimated by the model. Clearly, more testing is desirable and as noted earlier a comprehensive field program has been initiated to provide appropriate data. Additional model testing was recently reported for conditions of aldicarb use in Florida citrus production (Jones et al., 1983) and for other uses in Wisconsin (Jones, 1983). Figures 7–8 demonstrate the results obtained in those studies.

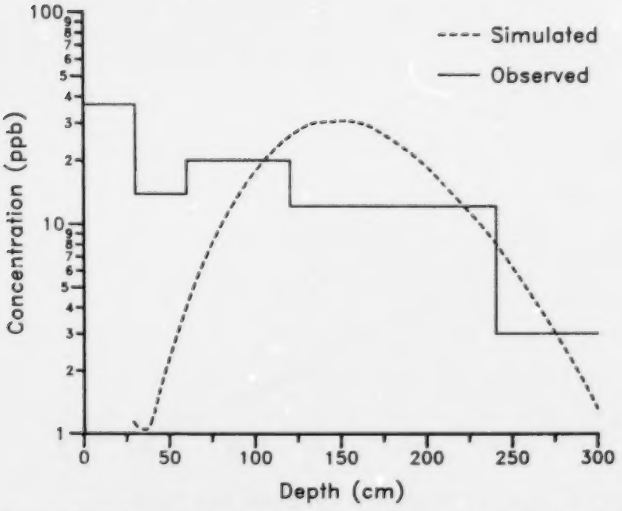

Fig. 8. PRZM test results for aldicarb use in potato production (after Jones, 1983).

MODEL APPLICATIONS

Generalized, time-varying simulation models of environmental systems are necessarily a compromise between a complete description of each microscopic process level detail and an adequate representation of the major processes sufficient to meet modeling objectives. Development and testing of the PRZM model is guided by the planned application of the model to investigate pesticide leaching potential under field crop conditions. More specifically, estimates of the probabilities of pesticides leaching below the plant root zone are desired.

The use of continuous simulation models to generate time series data is an accepted technique to derive probability statements about hydrologic events. Similarly, pesticide fate and transport models have been used to estimate probabilities of environmental exposure expressed as frequency distributions of concentrations in surface waters (Onishi et al., 1982; Donigian et al., 1983; Mulkey and Falco, 1983). Frequency distributions of the mass of pesticides leaching from the plant root zone appear to be valuable tools to assist in assigning relative risks of pesticide use. Specifically, they can be used in a question format, such as, what is the frequency of 10% of the annually-applied pesticides leaching below the root zone over a 20-year period of continuous use? PRZM can be used to answer the question by simulating a 20-year time period at a specific location and or a specific

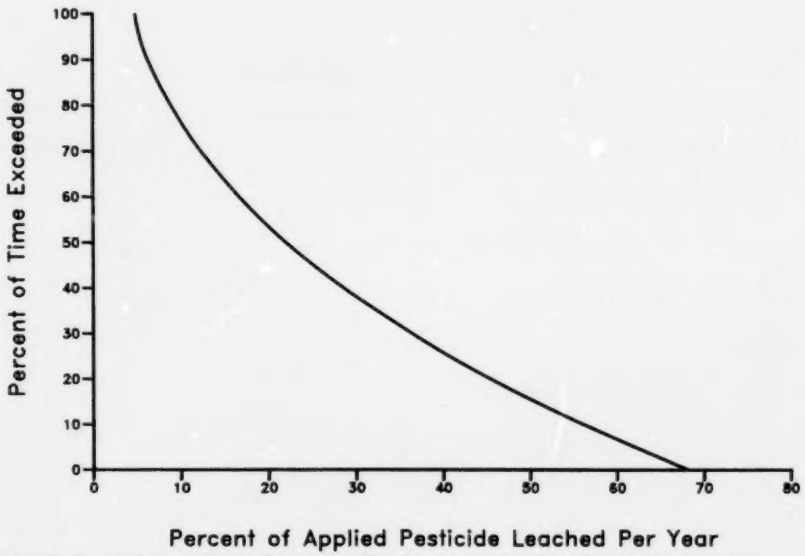

Fig. 9. Example cumulative frequency distribution evaluation of pesticide leaching.

pesticide. An example for a hypothetical pesticide having a degradation rate constant of $k = 0.01$ day^{-1} and a partition coefficient of $k_p = 0.01$ l/mg applied to wheat in Nebraska is given in Fig. 9. Because time series data are generated by PRZM, the plot in Fig. 9 is but one of many different ways to present the modeling results. Ultimately, additional model performance testing will suggest perhaps the optimum (more nearly accurate) format to display the model outputs. Experience to date suggests that mass fluxes rather than concentrations are the most appropriate values for extrapolation and interpretation relative to potential ground water threat.

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